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Ultralow-velocity zone geometries resolved by multi dimensional waveform modeling.

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5 6 **Ab**

6 Abstract 7 Ultra-low velocity zones (ULVZs) are thin patches of material with strongly reduced 8 seismic wave speeds situated on top of the core-mantle boundary (CMB). A common 9 phase used to detect ULVZs is SP_dKS (SKP_dS), an SKS wave with a short diffracted P 10 leg along the CMB. Most previous efforts have examined ULVZ properties using 1D 11 waveform modeling approaches. We present waveform modeling results using the 12 2.5D finite difference algorithm PSVaxi allowing us better insight into ULVZ 13 structure and location. We characterize ULVZ waveforms based on ULVZ elastic 14 properties, shape, and position along the SP_dKS raypath. In particular, we vary the 15 ULVZ location (e.g. source or receiver side), ULVZ topographical profiles (e.g. 16 boxcar, trapezoidal, or Gaussian) and ULVZ lateral scale along great circle path (2.5°, 17 5° , 10°). We observe several waveform effects absent in 1D ULVZ models and show evidence for waveform effects allowing the differentiation between source and 18 19 receiver side ULVZs. Early inception of the SP_dKS/SKP_dS phase is difficult to detect 20 for receiver-side ULVZs with maximum shifts in SKP_dS initiation of $\sim 3^{\circ}$ in epicentral 21 distance, whereas source-side ULVZs produce maximum shifts of SP_dKS initiation of 22 $\sim 5^{\circ}$, allowing clear separation of source- versus receiver-side structure. We present 23 a case study using data from up to 300 broadband stations in Turkey recorded 24 between 2005 and 2010. We observe a previously undetected ULVZ in the southern Atlantic Ocean region centered near 45° S, 12.5°W, with a lateral scale of \sim 3°, V_P 25 26 reduction of 10%, Vs reduction of 30%, and density increase of 10% relative to 27 PREM. 28

29 1. Introduction

30

Ultra-low velocity zones (ULVZs) are thin layers (typically less than 20 km

31 high) located on top of the CMB characterized by significant S and P wave velocity

- 32 decreases on the order of tens of percent. Several studies have also detected a
- 33 strong density increase on the order of 10% in ULVZs [e.g. Garnero and Jeanloz,
- 34 2000; Rost et al., 2005; Idehara 2011]. ULVZs seem to be regional features of the
- 35 lowermost mantle with many areas probed showing no evidence for ULVZ structure
- 36 [see McNamara et al, 2010 for review]. Several studies note ΔV_P to ΔV_S ratios of 1:3
- 37 which has been interpreted as evidence for a partially molten origin [Williams and

38 Garnero, 1996; Berryman, 2000; Hier-Majumder, 2008] with evidence for internal 39 structure due to melting processes [Rost et al., 2006; Hier-Majumder, 2014]. Nonetheless, iron enrichment of (Mg,Fe)O might also lead to similar material 40 41 properties [Wicks et al., 2010; Bower et al., 2011] in addition to iron enrichment of 42 perovskite and post-perovskite [Mao et al., 2006]. Possible origins of iron 43 enrichment include core-mantle reaction products in the vicinity of the CMB [Knittle 44 and Jeanloz, 1991], subducted banded-iron formations [Dobson and Brodholt, 45 2005], and pockets of remnant ancient basal magma ocean [Labrosse et al., 2007]. 46 ULVZs may mark areas where mantle flow collects dense material [Hernlund 47 and Jellinek, 2010; Bower et al., 2011; McNamara et al., 2010; Nomura et al., 2011]. 48 Current geodynamic predictions indicate that ULVZs may preferentially align near 49 the edges of Large Low Shear Velocity Provinces (LLSVPs) [McNamara et al., 2010], 50 regions characterized by $\sim 3\%$ S-wave velocity reductions beneath the Pacific and 51 Africa [e.g., Garnero and McNamara, 2008; Lekic et al., 2012]. However, these 52 geodynamic predictions are based on compositionally derived ULVZs, whereas 53 recent efforts indicate that partially molten ULVZs are likely formed within the 54 interior of LLSVPs [Li et al., 2013]. ULVZs have been tenuously linked to hotspot 55 volcanism [Rost et al., 2005; Burke et al., 2008; Thorne et al., 2013a] and may play a 56 significant role in the formation of mantle plumes and possibly the formation of 57 large igneous provinces [e.g. Burke and Torsvik, 2004]. Because ULVZs may be a 58 controlling factor in the formation of large scale mantle and surface features, 59 determining the geographic location, geometry, and geophysical characteristics of

60 ULVZs are key to unlocking not only the cause of these structures but also the role61 ULVZs play in large scale mantle dynamics.

62 ULVZs have been identified seismically by a number of studies using probes 63 such as ScP, ScS, PcP, SKS, and SP_dKS/SKP_dS phases (for an overview of recent ULVZ 64 detections see McNamara et al., [2010]). Each of these probes has trade-offs 65 between the different ULVZ parameters, most notably between P- and S-wave 66 velocity reduction and thickness. The core reflected phases (e.g. ScP, PcP, ScS) 67 typically have good vertical resolution while sampling regional CMB structure; the 68 diffracted phases (Sdiff, PKKPdiff, and SPdKS) are able to sample large lateral CMB 69 areas with less vertical resolution. These tradeoffs can be reduced by combining 70 several probes sampling the same CMB location [Jensen et al., 2013]. 71 In this study we concentrate on characterizing the interaction of the SKS-72 SP_dKS/SKP_dS system (in the following denoted as SP_dKS) with ULVZ structures. 73 SPdKS forms a post-cursor to SKS due to a short P-wave diffraction along the CMB

74 when SKS reaches the critical P-wave ray-parameter at the CMB (See Figure 1). This

75 system is particularly sensitive to CMB structure and allows sampling of large

76 geographic areas [e.g. Garnero and Helmberger, 1995; Garnero and Helmberger,

77 1996; Garnero and Helmberger, 1998; Thorne and Garnero, 2004; McNamara et al.,

78 2010]. Most previous efforts have resolved ULVZ properties through 1D waveform

79 modeling of SP_dKS [Garnero and Helmberger, 1995; Thorne and Garnero, 2004; Sun

80 et al, 2012] although recently 2D and 3D waveform propagation techniques have

also been used [Helmberger et al, 1996; Ni et al, 2003; Rondenay et al., 2010;

82 Thorne et al, 2007; Thorne et al., 2013a,b; Jensen et al., 2013, Brown et al., 2015].

83 These studies have found ULVZ related waveform effects that are not detectable in 84 1D modeling such as a precursory phase to SKS due to a top side ULVZ conversion 85 [Thorne et al., 2013b], early inception of SP_dKS/SKP_dS [Rondenay et al., 2010], and a 86 secondary diffraction from the top of the ULVZ structure [Ni et al., 2003]. However, 87 the majority of previous 2D and 3D efforts concentrated on simple ULVZ models 88 such as boxcar shaped ULVZs located at the inception point of SP_dKS or along the 89 most sensitive portion of the diffracted path [Jensen et al., 2013, Thorne et al., 90 2013].

91 Recent geodynamic modeling shows that ULVZ morphology is dependent on 92 viscosity, density and convective vigor forming ULVZs with different shapes 93 including symmetrical or asymmetrical triangles (as seen in profile) or flat topped 94 structures with steep sides [e.g. Tan et al., 2002; Bower et al., 2010; McNamara et al., 95 2010, Hier-Majumder and Revenaugh, 2010]. In this study we model more realistic 96 ULVZ structures by expanding from simple boxcar models to include Gaussian 97 shaped and flat-topped trapezoidal structures of varying length. We also examine an 98 expanded set of ULVZ locations in order to cover variation in the interaction of the 99 diffracted P-leg with the ULVZ. We use a large dataset of synthetic ULVZ waveforms 100 to infer the properties of SP_dKS recorded at 300+ stations located in Turkey. We 101 detect a small, roughly 3º wide, ULVZ located in the southern Atlantic Ocean in the 102 vicinity of the African LLSVP. The improved modeling allows certainty of the 103 location of the ULVZ on the receiver side, with northeastern and southwestern 104 boundaries of the ULVZ being well defined.

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107 2. Synthetic Modeling Methodology

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109 We compute synthetic seismograms using the 2.5D rotationally symmetric, 110 finite difference code PSVaxi, which uses a ring source with an amplitude that depends 111 on the sine of the take-off angle to generate waveforms [Jahnke, 2009; Zhang et al, 112 2009; Thorne et al., 2013a,b]. We use a finite difference grid with 18433 grid points 113 in the lateral (defined by co-latitude) direction and 4608 grid points in the depth 114 direction that permits robust calculations of waveforms with frequencies up to ~ 0.5 115 Hz. With the chosen setup we are able to compute high frequency synthetics while 116 keeping the memory and CPU time requirement manageable to simulate a large 117 database of synthetic waveforms. We use a rotationally symmetric Earth model with a PREM background velocity model [Dziewonski and Anderson, 1981] and velocity 118 119 variations representing ULVZ structure in the lowermost 50 km of the mantle. 120 Synthetics are bandpass filtered between 0.04 Hz and 0.5 Hz for comparison with 121 real data. 122 Here we use the PSVaxi method to simulate the effects of the location, size, 123 and geometry of ULVZs on SP_dKS . To reduce the large parameter space (ULVZ 124 location, thickness, seismic velocity, density, and ULVZ shape) we restrict modeling to P- and S-wave velocity reductions of -10% and -30% respectively and a density 125 126 increase of +10% relative to PREM [Dziewonski and Anderson, 1981]. The height of 127 the ULVZ above the CMB (h) is set to 10 km or 20 km to be in line with common 128 ULVZ observations [e.g. Garnero and Vidale, 1999; Rost and Revenaugh, 2003]. The

129	general behavior of waveforms for 10 km thick ULVZs is the same for 20 km thick
130	ULVZs, so we restrict our discussion to models with 10 km height for brevity. The
131	source depth is set to 500 km with a location at 0° co-latitude and all structure is
132	rotationally symmetric around a pole passing through the source and the center of
133	the Earth. In the model setup, epicentral distance from the source is synonymous
134	with co-latitude. This parameter space configuration reduces the variable space to
135	the ULVZ shape, ULVZ length (W), and the location of the ULVZ (\emptyset) in co-latitude
136	(Figure 2).
137	We define three ULVZ shapes: (1) boxcar, (2) Gaussian, and (3) trapezoid, as
138	shown in Figure 2. The boxcar model (Figure 2a) has previously been applied in 2D
139	modeling [e.g. Rondenay et al., 2010; Thorne et al., 2013a, Thorne et al., 2013b] and
140	is defined as an ULVZ with a length of W and an edge closest to the source (hereafter
141	near edge) at ϕ_1 degrees co-latitude and a height (<i>h</i>) equal to 10 km as follows:
142	
143	h. An person
144	
145	Geodynamical modeling shows that a boxcar shaped ULVZ is not a realistic
146	
	geometry. Instead, we expect ULVZs to form more pile-like structures dependent on
147	geometry. Instead, we expect ULVZs to form more pile-like structures dependent on the density and viscosity of the ULVZ and the ambient mantle [McNamara et al.,
147 148	geometry. Instead, we expect ULVZs to form more pile-like structures dependent on the density and viscosity of the ULVZ and the ambient mantle [McNamara et al., 2010; Bower et al., 2011; Hier-Majumder and Revenaugh, 2010]. To simulate this
147 148 149	geometry. Instead, we expect ULVZs to form more pile-like structures dependent on the density and viscosity of the ULVZ and the ambient mantle [McNamara et al., 2010; Bower et al., 2011; Hier-Majumder and Revenaugh, 2010]. To simulate this more realistic ULVZ structure, we model a Gaussian shaped ULVZ and a flat topped
147 148 149 150	geometry. Instead, we expect ULVZs to form more pile-like structures dependent onthe density and viscosity of the ULVZ and the ambient mantle [McNamara et al.,2010; Bower et al., 2011; Hier-Majumder and Revenaugh, 2010]. To simulate thismore realistic ULVZ structure, we model a Gaussian shaped ULVZ and a flat toppedtrapezoidal ULVZ. The height of the Gaussian shaped ULVZ (Figure 2b) is defined as:

$$h_{ulvz}(\phi) = h\left(e^{-\left(\left(\phi_1 + \frac{W}{2}\right) - \phi\right)^2 / 2*\left(\frac{W}{2\pi}\right)^2}\right)$$

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152

Here h_{ulvz} is defined by a function dependent on the co-latitude (ϕ) in degrees where the maximum height of the ULVZ is *h* kilometers at the center point between the near edge (ϕ_1) and the end of the anomaly at *W* degrees away from the near edge. <u>Note that 2π is an arbitrary factor to reduce the Gaussian function at the edges.</u> The trapezoidal shaped ULVZ model (Figure 2c) is defined by the piecewise function:

$$h_{ulvz}(\phi) = h \left(e^{-\left(\left(\phi_1 + \frac{W}{4} \right) - \phi \right)^2 / \left(\frac{W}{2\pi} \right)^2} \right) \qquad \phi_1 \le \phi \le \phi_1 + W/4$$
$$h_{ulvz}(\phi) = h \qquad \phi_1 + W/4 < \phi \le \phi_1 + 3W/4$$
$$h_{ulvz}(\phi) = h \left(e^{-\left(\left(\phi_1 + \frac{3W}{4} \right) - \phi \right)^2 / \left(\frac{W}{2\pi} \right)^2} \right) \qquad \phi_1 + 3W/4 < \phi \le \phi_1 + W$$

158

159

160 The function defines a trapezoid with Gaussian tapered sides that are ¹/₄ of the

161 anomaly length and a flat top with thickness h above the CMB for the remaining $\frac{1}{2}$ of

162 the anomaly length. We do not explore more complex ULVZ geometries such as

asymmetric piles [e.g. McNamara et al., 2010; Rost et al., 2010; Cottar and

164 Romanowicz, 2012] in order to limit the model space.

We model ULVZs with three different lengths of 2.5°, 5°, and 10° (~150, 300,
and 600 km on the CMB respectively). The lateral extent of ULVZs is currently not

167 well-known, but the majority of studies indicate ULVZs are likely in this size range 168 [e.g., McNamara et al., 2010]. We note however that larger ULVZ lateral dimensions 169 are possible [e.g., Thorne et al., 2013; Cottaar and Romanowicz, 2012]. Because the 170 SP_dKS waveforms are sensitive to the location of the ULVZ along the ray path [e.g., 171 Rondenay et al., 2010, Thorne et al., 2013], for each model length and shape we also change the near edge location in 2.5° increments. We calculate waveforms for four 172 173 base models, (1) the background PREM model [Dziewonski and Anderson, 1981]. 174 (2) a 1D ULVZ model, (3) a model with a boxcar ULVZ across the entire source-side 175 region, and (4) a model with a boxcar ULVZ across the entire receiver side (Figure 176 4).

177 **3. Synthetic modeling results**

178 Our modeling reveals several waveform effects that have not been observed in previous studies. First, ULVZ presence leads to an early inception of SP_dKS with 179 180 the magnitude of the shift dependent on the sidedness of the ULVZ. That is, the 181 SP_dKS arrival is apparent at smaller epicentral distances than predicted by the 182 PREM model. A similar effect was noted by Rondenay et al., [2010]. Here we extend 183 these findings to show that the shift of the SP_dKS inception distance is larger for 184 ULVZs occurring on the source side of the ray path than for receiver-side ULVZs 185 (Table 1). Second, we describe an additional seismic phase $SPd_{top}KS$ and further 186 internally reflected ULVZ multiples that are generated and interfere with the SP_dKS 187 for finite sized ULVZs less than \sim 600 km wide (Figure 3). The strong waveform 188 variations induced by these additional seismic phases might be interpreted as 189 complicated ULVZ structure in 1D models. Third, the SPdKS travel-time and

190 waveform anomalies are primarily sensitive to ULVZs where the P_{diff} -inception point

191 is within or geographically near (within 10°) the ULVZ. Long P-diffractions before

192 the interaction with the ULVZ structure lead to PREM-like waveforms. For finite

193 ULVZs along a long diffraction path minor travel-time variations of SP_dKS are

194 observable, but these variations are below the travel time resolution level of

195 recorded data. In the following, we will discuss these results in more detail.

196 **3.1. Source vs. Receiver Side ULVZs**

197 A key difficulty in determining ULVZ position using SP_dKS waveforms is the 198 inherent ambiguity between source- and receiver-side signals. 1D modeling 199 methodologies produce identical results for source or receiver side signals and 200 likely overpredict the amplitudes of ULVZ related phases [Thorne et al., 2013]. 201 Consequently, studies exploiting this phase often assume ULVZ location based on 202 other information such as crossing ray paths or additional information such as 203 proximity to LLSVPs [e.g. Garnero and Helmberger, 1995; Garnero and Helmberger, 204 1996; Wen and Helmberger, 1998; Thorne and Garnero, 2004; Jensen et al., 2013]. 205 Here we explore whether 2D modeling can be used to remove this ambiguity in 206 source versus receiver side structure.

Most previous 1D and 2D waveform modeling studies have focused on 1D ULVZ layers or large boxcar shaped ULVZs [e.g. Ni et al. 2003; Rondenay et al. 2010]. Observations from these studies include: (1) early inception of SP_dKS relative to the inception of SP_dKS of non-ULVZ models (e.g. PREM), (2) change of the move out of ULVZ sampling SP_dKS compared to non-ULVZ SP_dKS, (3) a SKS precursor phase for SKS directly striking an ULVZ resulting in a S-to-P conversion at the entry point of 213 the ULVZ [Thorne et al., 2013b] (referred to as SPKS in Fig. 3), and (4) additional SKS coda phases that can be categorized as diffractions along the top of the ULVZ (214 215 SptopPKS in Fig. 3). In this study we generate models for finite sized ULVZ models 216 that are either located at the SKS entrance/exit point at the CMB or sample the ULVZ 217 somewhere along the P-diffracted path of SP_dKS. We calculate synthetic traces for 218 epicentral distances of 90° to 130° (Figure 4). The expanded model space permits 219 clear detection of internally reflected ULVZ multiple phases (Figure 3). Full data 220 tables and waveform examples are included in the Supplementary material 221 (Supplementary Tables 1-9; Supplementary figures 1-36). 222 We establish our baseline by computing synthetic seismograms for the PREM 223 velocity model using PSVaxi (Figure 4a); three primary phases of interest, SKS, 224 SKS_{df}, and SP_dKS, are labeled. The SKS arrival time appears before zero because we 225 use a modified PREM model where we smooth the discontinuous jumps in seismic 226 velocity in the upper mantle. This is done to reduce the number of interfering 227 seismic arrivals in our wavefield. We plot waveforms aligned by the theoretical SKS 228 arrival time for an unmodified PREM model. All subsequent models discussed in this 229 manuscript are compared to this baseline calculation. 230 To explore the effects of 1D vs 2D models we initially run three models: (1) a 1D 231 ULVZ model (Figure 4b), (2) a source-sided ULVZ model (Figure 4c), and (3) a 232 receiver-sided ULVZ model (Figure 4d). The ULVZ models all consist of a 10km thick 233 ULVZ with a 10% drop in V_P , a 30% drop in V_s , and a 10% increase in density 234 relative to PREM. Note that waveforms and beyond 120° are dominated by the sPPP 235 phase labeled in (Figure 4a); SKS and SP_dKS waveform analysis beyond this distance 236 is therefore not considered. The 1-sided models (Figure 4c-d) produce identical 237 waveforms with the expected SKS precursor and early inception of the SP_dKS phase 238 in line with previous studies (e.g. Ni et al., 2003; Rondenay et al., 2010). This 239 indicates that for very large ULVZs (>1000km) the sidedness of an ULVZ structure 240 cannot be determined from the SP_dKS waveforms alone. However, the one-sided 241 ULVZ model predictions differ from the 1D ULVZ model predictions in two distinct 242 ways. First, the absolute time shift between the PREM predicted (blue line in Figure 243 4) SKS arrival and actual arrival is significantly greater (\sim 1s) than the time shift 244 predicted by the one-sided models. Second, the amplitudes of the ULVZ related 245 phases, namely the SPKS precursor and SP_dKS/SKP_dS arrivals, are amplified in the 246 1D model by approximately 200% implying that 1D models in general overestimate 247 the SP_dKS amplitude.

248 While it may not be possible to determine the location of the ULVZ at the source-249 or receiver-side of the ray path for large-scale ULVZ structures, our synthetic 250 modeling indicates that it is possible to determine the ULVZ position for smaller 251 scale ULVZs (i.e. for ULVZs less than \sim 600 km in length). Figure 5 shows synthetic 252 waveforms for a 5° (300 km) wide ULVZ with its near edge located at 15° (source 253 side) or 92.5^o (receiver side) co-latitude for each of the 3 ULVZ shapes (boxcar, 254 trapezoid, Gaussian). Since the SP_dKS raypath will encounter a source or receiver 255 sided ULVZ in the same way (Figure 4), one would expect these waveforms to 256 behave similarly for finite sized ULVZs, i.e. whether the ULVZ lies on the source- or 257 receiver-side of the model would be irrelevant. However, the waveform behavior for 258 the same model type is significantly different with respect to source-versus

259 receiver-side ULVZ locations (Figure 5). The source-side ULVZ models all contain a 260 phase which first appears at an epicentral distance of $\sim 97^{\circ}$ with a ray parameter 261 similar to the SP_dKS phase (<1s/^o relative to SKS_{ac}, indicated by the solid red line in 262 Fig. 5a-c). This phase is not observed for ULVZs solely located on the receiver-side. 263 This phase is also sensitive to the shape of the ULVZ. The largest amplitude arrivals 264 are observed for the boxcar model, whereas this arrival is only weakly observed for 265 the Gaussian models (Figure 5c). The trapezoid shaped models generate waveforms 266 intermediary in amplitude between the Gaussian and boxcar models. This waveform 267 behavior indicates that this phase is likely generated at the top of the ULVZ. Based 268 on the traveltime and slowness of the phase one potential candidate is the ULVZ 269 multiple phase SstopPKS (blue line in Figure 3) where the phase reflects off the CMB 270 the energy then reflects off the top of the ULVZ before propagating the remainder of 271 the path similar to the SKS phase. This secondary phase (solid red line in Figure 5) 272 interferes with the diffracted signal related to the top of the ULVZ, the SsP_dKS phase 273 identified by Rondenay et al. [2010] (red dashed line in Figure 5); the two phases 274 denoted by the red lines in Figure 6 destructively interfere to the point of 275 eliminating all signal between 116°-118° epicentral distance. The interference is 276 best observed in the boxcar models. This implies that if data are limited to this 277 narrow band of distances the secondary phases are no longer useful for ULVZ 278 identification.

The receiver-side ULVZ models do not contain SstopPKS but do contain an
additional arrival not present in the source-side ULVZ models. The additional arrival
for receiver-side ULVZ models behaves similar to a point diffraction with a ray

282 parameter much greater than SP_dKS . The origin of this phase can be related to 283 phases internally reflected within the ULVZ. The full waveform is produced by the interaction of the SKS with the ULVZ, which is quite different on the source and 284 285 receiver side due to the ray path geometry; on the receiver side direct interaction 286 between the SKS wavefield and the ULVZ is limited to rays spanning only a few 287 degrees epicentral distance (Figure 6). On the source-side the SKS core-entry points 288 are closely packed together leading to a waveform behavior closer to that expected 289 from a 1D ULVZ model whereas the SKS exit points sample a significantly larger 290 amount of area along the CMB and <u>only a small distance range is influenced</u> by 291 small-scale ULVZs (Figure 4). This stretching of the wavefront at the receiver side 292 might lead to the effect that the small-scale ULVZ acts as a point scatterer. The 293 behavior of the secondary phases demarked by the red line in Figure 5(c-e) for 294 receiver side ULVZ synthetics in combination with the fact that these phases have 295 not been observed in recorded data may indicate that the point scatterer behavior 296 occurs but is masked in real data by <u>3D</u> wavefront healing <u>effects</u>. It is important to 297 note that the SP_dKS arrivals alone are essentially identical for the source- and 298 receiver-side structure; this implies that identification of the additional phases 299 discussed above may provide a diagnostic tool for determining the location of ULVZ 300 structures.

These SKS coda phases (solid red line in Figure 6) are pervasive in the entire model set tested in this study. Yet, these phases have not been identified in any study to date. The elusiveness of these phases can likely be attributed to several factors. Within the epicentral distances of interest (105°-120°), these codas phases 305 occur significantly later in time (between 5 and 20 s after the SKS arrival). Thus, 306 these coda phases are likely outside the time window of interest traditionally used 307 to study SP_dKS waveforms. When the coda phase is developing for ULVZs close to 308 the theoretical inception point of SP_dKS it can either mimic SP_dKS (source side) or 309 interfere with the observable SPdKS phase (source and receiver side) (Figure 6 and 310 Supplementary Figures). The possibility for future detection of these coda phases 311 and their analysis to resolve the source-receiver side ambiguity for ULVZs lies with 312 very large aperture arrays such as USArray allowing dense sampling of the CMB exit 313 points or an "array of arrays" approach using multiple dense medium aperture 314 arrays that may be capable of producing large epicentral distance sampling along 315 similar backazimuths essentially reproducing the synthetic source-receiver 316 geometry of the synthetic data.

317 3.2. SKS precursors

318 ULVZs generate precursory energy stemming from an S to P conversion as 319 the wavefield enters the ULVZ, with a phase nomenclature of SPKS/SKPS for 320 source/receiver side conversion points (e.g. Ni et al., 2003; Rondenay et al., 2010; 321 Thorne et al., 2013). This phase is particularly important in resolving ULVZ location 322 as the down-going (up-going for receiver-side ULVZ) S-leg of the SPdKS raypath 323 must intersect the ULVZ to generate this phase. For a 1D ULVZ model with a ULVZ 324 thickness of 10 km this precursor is observed across all sampled epicentral 325 distances (Figure 4). However, for finite length ULVZs the shape of the ULVZ 326 determines the waveform behavior of the precursor (Figure 6, also see 327 Supplemental Figures 1-36). Synthetics from this study indicate that ULVZs with a

328 length less than 2.5° (~150 km) do not produce a detectable precursor phase 329 regardless of the ULVZ shape (Table 1 and Supplementary Figures 1-36). Moderate 330 sized ULVZs with a length of 5° (~300 km) or 10° (~600km) are capable of 331 producing the precursory phase, but are more detectable for flat topped structures, 332 likely due to defocusing effects associated with Gaussian shaped structures. The 333 precursor is not a significant phase for 5° or 10° wide Gaussian shaped ULVZs 334 (Table 1 and Supplementary Figures 1-36). The observability of this precursory 335 phase also depends on the location of the ULVZ on source or receiver due to the 336 different sampling of the wavefield. Consequently, the precursor for a receiver sided 337 10° wide ULVZ is only detectable over ~5-6° of epicentral distance across the 2D 338 synthetic array whereas the same source-sided ULVZ produces a precursor over a 339 larger (>10^o) epicentral distance ranges (Table 1, Supplementary Figures 1-36). The SKS precursor phase, is most detectable for source-side, flat-topped ULVZ structures 340 341 more than 150 km wide. The epicentral range at which the precursor is detectable is 342 dependent upon the location of the ULVZ with respect to the SKS wavefield as well 343 as the shape of the ULVZ (See Supplemental Figures 1-36). On the other hand, the 344 limited epicentral distance range that allows ULVZ precursor observation on the 345 receiver side indicates that this phase would be difficult to identify in recorded data. 346 **3.3. SP**_dKS inception point

For the PREM model, the bifurcation of SP_dKS from SKS is noticeable in
waveforms beginning at an epicentral distances of ~110°, but the inception of SP_dKS
for the PREM velocity model theoretically occurs as early as ~104° [Thorne and
Garnero, 2004]. The presence of an ULVZ near the theoretical inception point of this

351 phase generates an observable bifurcation of the SP_dKS phase at shorter epicentral 352 distances than predicted by PREM. The distance at which this bifurcation is 353 observable is primarily influenced by the ULVZ P-wave velocity [e.g. Rondenay and 354 Fischer, 2003]. The models shown here indicate a similar behavior, but highlight a 355 critical difference between source- and receiver-side ULVZ locations. For source-356 side ULVZs wider than ~150 km the largest observed epicentral distance shift in the 357 bifurcation is $\sim 5^{\circ}$ with observable SP_dKS arrivals starting at $\sim 104.5^{\circ}$. In contrast, 358 the receiver side equivalents have a maximum shift of $\sim 3^{\circ}$, but more often the 359 bifurcation shift is not observable due to interference from secondary phases (e.g. 360 SsP_dKS) or have a shift of less than 1^o (Table 1, Supplementary Figures 1-36). Such 361 small changes of the inception point are likely not observable in sparsely populated 362 record sections, yet large values of the shift in bifurcation distance may indicate 363 ULVZ presence on the source-side of the ray path.

364 3.4. Diffraction Length and ULVZ detectability

365 The length of the diffracted leg along the CMB increases with epicentral distance 366 (Figure 5). Because the diffracted path integrates over the velocity structure along 367 the path, only shorter paths associated with SP_dKS data less than $\sim 120^{\circ}$ epicentral 368 distance show measurable travel time and waveform effects due to ULVZ interaction 369 in recorded data (see Supplementary Material). Waveforms of SP_dKS recorded at 370 distances larger than $\sim 120^{\circ}$ in general resemble PREM waveforms. To determine 371 the sensitivity of each synthetic model for the detection of ULVZ structure along the path, while attempting to minimize the influence of the secondary phases we cross-372 373 correlate the model waveforms with those produced for the PREM base model over

374 a 20 second window centered about the SKS arrival. Figure 7 shows the results of 375 this analysis for 10° wide ULVZs with a thickness of 10 km; any correlation co-376 efficient larger than 0.85 is considered undistinguishable from PREM. For both 377 receiver and source side ULVZs, boxcar shapes are the most detectable whereas 378 Gaussian shaped ULVZs are the least detectable based on the limited size of the 379 detectable correlation coefficient footprint (Figure 7). Detectable source side ULVZs 380 have the near edge located at no more than 15° co-latitude. Source side ULVZs are 381 also detectable over a wider range of distances (more than 5^o epicentral distance) 382 whereas receiver side ULVZs are only detectable over a narrow (less than 5°) 383 epicentral distance corridor (Figure 7a,c,e). This implies that source-side ULVZs are 384 easier to detect using the SPdKS phase. Receiver side ULVZs are most detectable for 385 ULVZs located with a near edge between 87.5° and 92.5° ; the strong secondary 386 "point diffractor"-like phase discussed in the previous sections generates the key 387 correlation signals at larger distances (Figure 7b,d,f). The limited regions defined by 388 correlation coefficients in which an ULVZ is detectable using the SP_dKS system 389 further implies that imagining ULVZs requires specific source receiver geometries in 390 order to be imaged partly explaining the many non-observations in SP_dKS data. The 391 SP_dKS phases generated by ULVZ models with these specific material properties and 392 thickness outside the co-latitude limits described above would likely be 393 indistinguishable from PREM SPdKS phases especially in the presence of noise in 394 recorded observations. 395 Consequently, this implies that it will be virtually impossible to image source side

396 ULVZs sampled only by SPdKS with stations at distances larger than $\sim 115^{\circ}$

epicentral distance. For receiver side ULVZs SP_dKS data become more complex at
large epicentral distances. While SP_dKS itself behaves identically to the source side
SP_dKS, the secondary phase for models with a near edge between 100° and 105° colatitude actively interferes with SP_dKS arrivals for seismic traces between 115° and
120° epicentral distance (See Supplemental Figures). Therefore the newly observed
late phases (Ss_{top}PKS,Sp_{top}PKS) might be the key to further ULVZ detections at larger
distances.

404 One of the main observables based on these synthetics is the interaction of the 405 SKS phase with the top of the ULVZ rather than the SP_dKS phase itself (Figure 3.6. 406 Supplementary Figures). The interference of the energy produced by this 407 interaction with the SP_dKS results in reduced detectability of the early bifurcation 408 and generates strong secondary phases with a significantly different ray parameter 409 for receiver side ULVZs (red lines in Figure 6). This indicates that ULVZs less than 410 600km wide have different source/receiver side characteristics and secondary 411 phases may be applied to ascertain the sidedness of an ULVZ.

The extensive modeling of this study highlighted several unknown waveform
effects allowing better characterization of ULVZ properties. Using waveform
information it might be possible to identify the shape of ULVZs which is important
for understanding the dynamics of ULVZs at the CMB (Bower et al., 2011). Using
later arriving phases it might be possible to identify the exact location of the ULVZ
along the raypath and resolve the inherent ULVZ source-receiver side ambiguity of
SP_dKS.

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420

421 **4. ULVZs at the southern edge of the African Superplume.**

The synthetic modeling presented in the previous sections indicates that the
SKS/SPdKS system generates a distinct fingerprint for a given ULVZ location, size
and geometry. We apply these findings to a new dataset using stations in Turkey
that provides us with CMB sampling in the vicinity of the northern edge of the
African Large Low Shear Velocity Province (LLSVP) that has not been probed for
ULVZ structure before [see summary of previous ULVZ observations in McNamara
et al., 2010].

429 Recent large-scale deployments of seismic stations across Anatolia provide a 430 well-suited dataset to study how the waveform behavior of finite sized ULVZs 431 observed in the 2.5D synthetics may be applied to determine ULVZ location, elastic 432 parameters and geometry. We use broadband data from station deployments of the Kandilli Observatory and Earthquake Research Institute Network (IRIS network 433 434 code: KO), the Turkish National Network (TU), the PASSCAL North Anatolian Fault 435 experiment (YL), and available data from European networks available via Orfeus 436 (http://www.orfeus-eu.org) from 2005 to the middle of 2010. The resultant dataset 437 consists of 449 individual stations comparable in size to the USArray network albeit with less regular station spacing. The combination of these networks provides a 438 439 large aperture array with sufficient data coverage to analyze SKS and SP_dKS/SKP_dS 440 waveforms generated by deep focus events in South America, the South Sandwich 441 Islands and the West Pacific (Figure 8). This dataset, especially waveforms from

442 events in the Americas, sample the CMB in the proximity of the northern edge of the 443 African LLSVP upon exit from the core (Figure 8) [Grand, 2002; Garnero and 444 McNamara, 2008; Lekic et al. 2012] as well as CMB areas beneath South America, 445 the Caribbean, the southern Atlantic, western Pacific and western Asia. Due to 446 station locations the northern and western boundary of the African LLSVP is not 447 well sampled despite efforts from previous work using events from both the South 448 Atlantic and Africa [e.g. Helmberger et al., 2000; Ni and Helmberger, 2001; Ni and 449 Helmberger, 2003]. Many of the regions sampled in this study are either new or are 450 areas where previous work indicates a mix of ULVZ detections and non-detections 451 in individual studies, for example beneath South America.

452 In our data analysis we follow the approach presented in Thorne et al. 453 [2013b] with one key difference, for this data set we make no assumption on which 454 side of the ray path the ULVZ exists on prior to analysis. Raw data are first 455 transferred to a displacement signal using available pole-zero metadata and 456 bandpass filtered to frequencies between 0.04 Hz and 0.5 Hz. We limit our data to 457 events with earthquake depths larger than 100 km and select events with simple 458 source-time functions. Additionally, we require that there is data coverage for each 459 event between 90° and 100° epicentral distance such that a source time function 460 can be constructed and subsequently deconvolved from the time series to permit 461 combining data from multiple events. Here we are assuming that any possible 462 waveform distortion between 95^o-100^o will be eliminated by the stacking process. 463 This selection leads to a total usable data set of 29 events. We deconvolve the source 464 from the data by using the stacked SKS waveform for epicentral distances less than

465 100° as an estimate of the source wavelet and apply a water-level deconvolution 466 with a k-value equal to 0.2 [Clayton and Wiggins, 1976]. We next grid the data into 2.5° by 2.5° geographic bins based on SPdKS inception points (the point where P-467 468 diffraction initiates on the CMB) for all source and receiver regions containing at 469 least one 5° by 5° square with a minimum 100 inception points (Figure 8, 9, 10). 470 This results in four source-side regions with dense data coverage beneath: (1) South 471 America (Figure 9a), (2) the Caribbean (Figure 9b), (3) the South Sandwich Islands 472 (Figure 9c) and (4) the West Pacific (Figure 9d). These regions sample a wide 473 variety of mantle environments from subduction dominated regions (Figure 9a, b) 474 to LLSVP border regions (Figure 9c,d) [Grand, 2002]. The receiver side inception 475 points sample: (1) the northeast corner of the African LLSVP beneath the 476 Mediterranean (Figure 10a) and (2) what appears to be more normal mantle beneath continental Eurasia (Figure 8, 10b). As we make no a-priori assumption as 477 478 to the probable location of any ULVZ, each region is analyzed individually. For each 479 geographic bin the data are stacked in 1º epicentral distance bins and cross-480 correlated with approximately six-hundred 2.5D synthetic waveform models (see 481 Table 2 for details). To account for the high frequency content of our 2.5D models. 482 we run multiple sets of cross-correlations for each bin with the synthetic data 483 bandpass filtered between 0.04 Hz and 0.5 Hz as well as synthetic data bandpass 484 filtered between 0.04 Hz and 0.2 Hz. In practice, the dominant period of the observed waveforms is on the order of 5-10s. 485 We determine the best-fit model by finding the maximum mean cross-486 487 correlation coefficient for geographic bins containing a minimum of five 1°

epicentral distance binned waveforms and more than 15 individual waveforms
(Figure 11). We run cross-correlations for the time window between 10 s before
SKS to 20 s after SKS to account for the possible presence of SP_dKS for each
individual binned trace before calculating standard statistics for the record section,
including the mean, standard deviation, median, quartiles, minimum, and maximum
correlation coefficient.

494 To determine if this best fit model provides a better fit than PREM, we apply 495 multiple metrics. For each individual $2.5^{\circ} \times 2.5^{\circ}$ geographic bin we first apply a 496 cross-correlation cutoff. If the mean correlation coefficient between 1° epicentral 497 distance data stacks and synthetics for the PREM waveforms is greater than 0.78 498 then the bin is classified as PREM-like. Waveform inspection indicates that PREM-499 like and ULVZ-like waveforms are essentially indistinguishable for mean correlation 500 coefficients larger than 0.78. We therefore assume that if the mean correlation 501 coefficient is less than 0.78 the geographic bin possibly contains ULVZ structure. We 502 next compare data stacks to the synthetics generated for our suite of ULVZ models. 503 We next determine which ULVZ model provides the best-fit (based on mean cross-504 correlation coefficient). If the best-fit model has a mean cross-correlation greater 505 than PREM's mean cross-correlation plus 1 standard deviation, then we further 506 consider the bin to be possibly ULVZ-like. Considering only simple standard 507 deviations when comparing model fits often results in overlapping or near 508 overlapping <u>values</u>. For example, the South American grid node SA_E10 (Figure 9a, 509 11) has 165 individual seismograms over all 17 epicentral distance bins (104^o-510 120°). The cross-correlation results for the 0.04-0.2Hz bandpass filtered data

511 indicate that a boxcar ULVZ with a length of 10° located 5° away from the source 512 would be the best-fit model with an average cross-correlation coefficient of 513 0.76±0.10. Comparable PREM models reach cross-correlation values of 0.71±0.05. 514 The PREM model does not reach the minimum cross-correlation coefficient and the 515 ULVZ model has a higher average correlation coefficient. The ULVZ model would 516 therefore move on to the next step in analysis based on the raw numbers of the 517 mean correlation coefficient, but it is important to note that the standard deviations 518 of the two models do overlap. Given that we are examining a population with only a 519 small change in the measure of fit, correlation coefficients, a simple confidence 520 about the mean is not the best measure to compare the models. To determine the 521 quality of a fit of waveforms for PREM vs. an ULVZ model a better metric is required 522 than simple mean comparison. In this analysis we pass these type results into the 523 visual inspection process. The development of a robust statistical metric to be 524 applied in lieu of or in conjunction with the mean is a venue for future study. 525 Waveform matches for the South American grid E10 for both the PREM 526 (Figure 11b) and the best-fit ULVZ model (Figure 11c) are shown in Figure 11; the 527 most substantial mismatch is due to slight differences in the frequency content of 528 the 2D models. Critically, these data (black lines in Figure 11) do not have a clear 529 SP_dKS phase at 110^o epicentral distance as required by the best-fit ULVZ model 530 (Figure 11b). Indeed, the worst fitting portion of the ULVZ model is between 109°-114° epicentral distance where the sensitivity to the model ULVZ is greatest. The 531 532 ULVZ model, however, does better match the timing of the observed SP_dKS arrival 533 between 114-117^o. A conservative interpretation would err towards a null

534 detection whereas a less conservative interpretation based on timing match 535 between 114°-117° of the SPdKS arrival would detect evidence for a ULVZ. In this 536 case we mark the result as inconclusive/possible ULVZ; the dashed white lines in 537 Figure 9 outline the possible ULVZ regions. It is worth noting that this particular 538 example is an extreme borderline case between ULVZ detection and non-detection 539 and as with any human based method open to interpretation. Here we elect to be 540 extremely conservative only interpreting ULVZ detections if there is a clear early 541 inception of the SP_dKS phase in the data. This minimizes the possibility of false 542 positives, but may eliminate detections of subtle ULVZ structure. 543 We observe a similar situation for the Mediterranean receiver side grid node D4 (MED_D4) (Figure 10a, 11d-f). Here the PREM model has a mean correlation 544 545 coefficient of 0.77±0.03 whereas the best-fit ULVZ model, a 10^o long boxcar with a height of 10km, V_P reduction of 10%, V_S reduction of 30%, density increase of 10%, 546 547 and left-edge location 5° from the source, has a mean cross-correlation coefficient of 548 0.81±0.10. As with the South American grid node SA_E10, there is significant 549 mismatch between the observed inception point of the SP_dKS and the ULVZ model, 550 and a better timing match of the SP_dKS arrival at larger epicentral distances 551 between 114-118° (Figure 11d-f). Interestingly, this receiver side grid node 552 indicates a preference for a source-side ULVZ beneath South America in the similar 553 location as the ULVZ modeled in SA E10 with the same properties. As with the 554 former case for SA_E10, the more conservative interpretation of no ULVZ/possible 555 ULVZ is preferred.

556 The data analysis method presented here has the advantage that the first 557 two numerical analysis tests, PREM correlation coefficient cutoff and mean test can 558 be performed automatically. This reduces the number of required visual inspections 559 for large datasets. However, as the example for SA_E10 and MED_D4 indicates, the 560 visual inspection is still a critical step for determining whether a confirmed ULVZ 561 model is warranted for a given dataset.

562 The data analysis in this study uses extremely stringent requirements to 563 obtain a positive identification of an ULVZ. Consequently, the majority of the results 564 do indicate PREM-like CMB structure. Due to the restricted size of our synthetic 565 model library there may be some cases where a ULVZ structure is probable, but the 566 current model library does not contain the correct parameters or the diffracted path 567 sampling is not sufficient to determine ULVZ structure. It is important to note that this method is essentially a grid search of forward models; the method's 568 569 effectiveness is dependent upon the completeness of the library. An expanded 570 model library may be able to find an ULVZ model match for some grid nodes 571 assigned a PREM value, but given the required computation time for a single model 572 $(\sim 36-72$ hours per model using eight 2GB processes on the ARC1 parallel cluster 573 based in the University of Leeds which uses Intel X5560 2.8GHz processors or eight 574 <u>2GB processes on a single computer with 32Gb RAM and an Intel quad core</u> 575 processor) a complete ULVZ SPdKS waveform library with variations in ULVZ height, 576 velocity, and density requires significant time and commitment and does not seem 577 feasible at the moment.

578 With these strict requirements for detection we do not identify ULVZs for the 579 South American, Caribbean, or West Pacific source-side geographic bins, but do 580 identify one ULVZ near the South Sandwich Islands (Figure 9) which is discussed 581 further below. All of the receiver-side geographic bins (Figure 10) do not contain <u>a</u> 582 detectable ULVZ structure. This majority null result that includes some borderline 583 cases such as the South American case (SA_E10) previously described is consistent 584 with the mixed and null results previously recorded in these regions [Idehara et al., 585 2007; Persh et al., 2001; Thorne and Garnero, 2004]. We do not detect the ULVZ 586 imaged by Zou et al. (2007) using PKP data within the South American grid. There 587 are two potential explanations for this seemingly contradictory observation: The 588 grid overlapping the region sampled by Zou et al. [2007] is the same region sampled 589 by the borderline case described for the South American grid E10; the null detection 590 could be the result of the very strict restrictions we apply to the automated 591 detection system, the misfit with a particular ULVZ model in the library and/or a 592 small scale ULVZ sampled by a minority of the diffracted paths. Nonetheless, our 593 results indicate that the waveform is most likely well explained by a PREM-like CMB 594 region.

595 The results using the strict cut-off and semi-automated detection do indicate 596 that there exists an ULVZ in the South Atlantic. The grid references SSI_D2, SSI_E2,

and SSI_E3 indicate that there is likely a $\sim 3^{\circ}$ wide boxcar shaped ULVZ

approximately 13^o away from the source location (Figure 12 and Supplementary

599 Figures 37-38). Figure 12 shows the modeling results for the South Atlantic Grid E2

600 (SSI_E2). Here the PREM model yields cross correlation coefficient of 0.74±0.11

601 (Figure 12a); the best-fit boxcar ULVZ model (Figure 12b) with a near edge location 602 of 13^o and length 3^o has a correlation coefficient of 0.87±0.07. Upon visual 603 inspection the ULVZ model successfully models the inception of SP_dKS at 604 approximately 108° epicentral distance (Figure 12b) whereas the PREM model does 605 not match the observed inception point. The model library applied in this case study 606 included Gaussian and trapezoid shaped ULVZs yet the best-fit model was a boxcar 607 shaped ULVZ. The best-fit Gaussian model with a near edge location at 12.5° colatitude and a length of 5° (~300 km) has a mean correlation coefficient of 608 609 0.84±0.07 while the best-fit trapezoid model with a near edge location at 10° co-610 latitude and length of 5° has a mean correlation coefficient of 0.82±0.08. While the 611 mean correlation coefficient is not significantly different for any of the model types, 612 the median correlation coefficients for the best-fit boxcar, Gaussian, and trapezoid 613 models are 0.87, 0.83, and 0.82 respectively indicating that the boxcar model is a 614 better fit for the overall dataset given the current models available in the model 615 library.

616 The significance of secondary phases was discussed and observed in the 617 earlier sections describing the synthetic results. The data here do not indicate a 618 clear secondary phase, but the data show small arrivals about 7-10 s after the SKS 619 specifically for distances of 104° and 108° - 116° (Figure 12). While the signal is not 620 strong enough to provide a positive identification it does indicate that searching for 621 the secondary reflections related to SKS may be possible. Such a search, however, 622 would require an event based analysis so that data between 90° and 104° could be 623 effectively analyzed.

624 The identification of this ULVZ structure is of particular interest as it is 625 located less than approximately 300 km off the southern edge of the African LLSVP 626 as indicated in tomographic images (Figure 8, 9c). While the detection of ULVZ 627 structure along the border of a LLSVP is not a new phenomenon, the majority of 628 ULVZ detections are primarily in the vicinity of the Pacific LLSVP [see McNamara et 629 al. [2010] for a review]. ULVZ structure detections in the vicinity of the African 630 LLSVP are significantly rarer partially due to less data availability to probe deep 631 mantle structures. There are a few ULVZ detections further north and south of our 632 detection [Rost et al, 2006; Wen, 2002]. Additional work has detected ULVZs and 633 low velocity structures in the South Atlantic using ScS and SP_dKS data approximately 634 10° north of our sampled location but the precise location of the ULVZ detected in 635 this study has not been probed previously [Helmberger et al., 2000; Ni and 636 Helmberger, 2001; Tkalčić and Romanowicz, 2002].

637

638 **5. Conclusions**

639 Most past studies of ULVZ structure have employed 1D methods to compute 640 synthetic seismograms in order to model ULVZ seismic properties (e.g. Sun et al., 641 2012; Avants et al., 2006; Garnero and Helmberger, 1995; Garnero and Helmberger, 642 1996; Garnero and Helmberger, 1998). Typically, an implicit assumption is made as 643 to whether the ULVZ is located at the source- or receiver-side of the SKS path. The 644 synthetic waveforms calculated in this study indicate that ULVZ structures less than 645 600 km wide create distinct waveform patterns that can be used to differentiate 646 between source- and receiver-side ULVZs. We show that a-priori information on

647 ULVZ location is not necessarily needed, but that such assumptions may also lead to the false identification and location of ULVZs. We have presented a case study using 648 a preliminary method to conduct a robust search for ULVZ structures using large 649 650 aperture arrays. Most of our study region seems to be ULVZ free or may contain 651 ULVZs below the detection threshold [Rost et al., 2010] giving more evidence to the 652 hypothesis that ULVZs are regional phenomena. We show evidence for ULVZ 653 structure in the South Sandwich Island region at the edge of the African LLSVP. The 654 best-fit model for this previously undetected ULVZ in the South Atlantic indicates a 655 steep sided ULVZ about 180 km across and 10 km high with a Vs decrease of 30%, VP 656 decrease of 10% and density increase of 10% relative to PREM. 657 It is important to note that the method applied here is essentially a grid 658 search over a library of forward models. Despite the fact that the library in this 659 study consists of hundreds of models, a more complete library of ULVZ models

660 including <u>additional</u> velocity, density, ULVZ height <u>parameter</u> variations is needed. <u>A</u>

661 more complete and robust synthetic library would permit directed searches when

662 <u>comparing synthetic waveforms with observations of the SPdKS system.</u> Currently,

663 depending upon the topology and computational processors available, a single

664 model requires between ~36 and 72 hours of runtime <u>using eight processes on the</u>

665 <u>ARC1 parallel computing cluster at the University of Leeds</u>. In order to generate a

666 complete model space, a community effort and funding for the generation, storage,

and data basing of available 2.5D models is needed.

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890891892 Figure Captions



- 894 Figure 1: Schematic diagram of the SKS (black dashed line) and SP_dKS/SKP_dS (gray
- 895 lines) ray paths. Note that the diffracted path of the SP_dKS/SKP_dS can occur on
 896 either the source or receiver side.



Figure 2: Schematic of the ULVZ models types, boxcar (a), Gaussian (b), and

trapezoid (c) used in this study in terms of co-latitude (\emptyset), ULVZ width (W), and

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ULVZ maximum height (*h*).





- 904 Figure 3: Schematic of phases that can be generated by an ULVZ including SPdKS
- 905 (green), the precursory phase SPKS (red), a diffraction along the top of the ULVZ
- 906 SPdtopPKS (black), and the internally reflected phases SstopPKS and SptopPKS (blue
- 907 and orange respectively).



- 908 909
- 910 Figure 4: 2.5D base models produced by PSVaxi for the smoothed PREM model (a), a 911 1D ULVZ covering the whole CMB (b), a large source sided ULVZ (c), and a large 912 receiver sided ULVZ (d). The schematics below (b), (c) and (d) denote the ULVZ 913 structure used to generate the waveforms. Significant structures are labeled 914 including the SKS precursor, and the SP_dKS/SKP_dS phases. Note that the waveforms 915 in (c) and (d) are essentially identical. The red line in 4c denotes the arrival of the 916 <u>SPKS precursory phase. Note that waveforms and beyond 120^o are dominated by</u> 917 the sPPP phase labeled in (a); SKS and SP_dKS analysis beyond this distance is

918 therefore not considered. A 1D ULVZ model calculated using the reflectivity code

- 919 *psquik* (after Müller, 1985) with the same ULVZ parameters is shown in the
- 920 <u>supplementary material (Supplementary Figure 41)</u>





Figure 5: A selection of waveform results for a 5° long ULVZ on the source side with
a co-latitude location L1=15° (top) and receiver side with L1=92.5° (bottom) for the
three different types of ULVZs, boxcar (a, d), trapezoid (b, e), and Gaussian (c, f).
Based on the geometry on the SPdKS raypath the top and bottom rows are expected
to be identical, but these synthetics show stark differences most notably the

- different inception point and ray parameter for the SKS coda phase as described in
- 928 the text.



929 Figure 6: Schematic of array model sensitivity for the SKS and SP_dKS/SKP_dS phases 930 for an ULVZ on the source (a) and receiver (b) side. Solid lines below the raypaths 931 represent the coverage of the diffracted path of the SP_dKS/SKP_dS ray paths for 932 933 epicentral distances of 110^o(blue), 115^o(yellow), and 120^o(red). Triangles and 934 squares represent the separation distance of SKS and SP_dKS/SKP_dS at the CMB and 935 the piercing point of SKS at the CMB, respectively. Note that the major sensitivity 936 differences between the source and receiver side stem from the piercing points of 937 the SKS phase rather than the SP_dKS/SKP_dS paths. 938





939 940 Figure 7: Results

940 Figure 7: Results from the cross-correlation between the seismograms produced by941 ULVZ models and the PREM model. The plots show the resultant correlation

942 coefficients for 10^o wide ULVZs located on the source side (a, c, e) and receiver side

943 (b, d, f) for each ULVZ shape modeled in this study, boxcar (a, b), Gaussian (c, d), and

944 Trapezoid (e, f). The dark blue regions indicate where the correlation coefficient

- 945 between the ULVZ synthetic seismograms and the PREM synthetic seismograms is
- 946 greater than or equal to 0.85. The regions with high correlation coefficients are
- 947 geometries where PREM and the ULVZ model would be indiscernible with the
- 948 addition of noise.



950 Figure 8: (a) Global station (triangles) and event (stars) distribution for the data

analyzed in the case study. The outline of the LLSVPs as indicated by the -1% Vs

952 contour of the tomographic model by Grand (2002) is shown as orange. All

953 SP_dKS/SKP_dS diffraction paths available for analysis using the stations and events

are also shown. Receiver side diffraction paths are shown in black; <u>source</u> side paths

955 are shown in blue. Boxes indicate areas shown in Figures 9 and 10.

965

966 Figure 9: Source side grids analyzed in the case study underlain by the S-wave

967 velocity perturbations at the CMB (Grand, 2002) the SP_dKS inception points are

968 plotted as crosses. The grid labels are shown along the north and western margins

969 for (a) the South American grid, (b) the Caribbean Grid, (c) the South Sandwich

970 Island Grid, and (d) the West Pacific Grid. The ULVZ identified in the case study is

shown in (c) by the red polygon. <u>The white dashed lines indicate the extent of other</u>
 possible but not confirmed ULVZs detected in the case study. Locations of areas are

9/2 possible but not commined ULV2s detected in the case study. Locations of areas are

973 indicated in Figure 8.

974 975 Figure 10: Same as Figure 9 but showing the receiver side grids for (a) the

- Mediterranean and (b) the continental <u>Eurasian</u> grid. Locations of areas are 976
- 977 indicated in Figure 8.

Figure 11: Example of waveforms for the South American grid node SA_E10 (a-c) 979 980 and the Mediterranean grid node MED D4. The data (black) are shown with 981 synthetic results for the PREM model (b/e, blue), the best fit ULVZ model (c/f, red), boxcar model with ULVZ location (source side) $L1=5^{\circ}$ and length W=10^{\circ}, and the 982 raw data (a/d). Synthetics are bandpass filtered between 0.04-0.2Hz. Most of the 983 984 mismatch between the waveforms can be explained by slightly differing frequency 985 contents between the synthetic and observed data due to the source deconvolution process and subsequent stacking or attenuation of the data SKS waveform. 986

Figure 12: Example of an ULVZ detection for the South Sandwich Island grid node
E2. The data (black) and stacks are shown in (a). (b) Datastacks (black) and
synthetic results for PREM (blue) and (c) datastacks (black) and the best fit ULVZ
model (orange). Synthetics were calculated for a boxcar model with ULVZ location
(source side) L1=13° and length W=3°. The data includes a clear inception of SPdKS

993 near 108º epicentral distance.

101(

Table 1: General characteristics of the synthetic 2D ULVZ models. "XX" indicates

1012 where the SP_dKS inception distance shift is not observable or is masked by

1013 interfering phases.

Shape	Length (º)	SRC/REC Side	Max SPdKS Inception Distance Shift (º)	SKS Precursor Observed? Y/N
Gauss	2.5°	SRC	1.5°	N
Trapezoid	2.5°	SRC	0.5°	Ν
Boxcar	2.5°	SRC	XX	Ν
Gauss	5°	SRC	5°	Ν
Trapezoid	5°	SRC	0.5°	Y
Boxcar	5°	SRC	5°	Y
Gauss	10°	SRC	4°	Y
Trapezoid	10°	SRC	5°	Y
Boxcar	10°	SRC	6°	Y
Gauss	2.5°	REC	0.5°	Y
Trapezoid	2.5°	REC	XX	Ν
Boxcar	2.5°	REC	XX	Ν
Gauss	5°	REC	1°	Ν
Trapezoid	5°	REC	0.5°	Y
Boxcar	5°	REC	XX	Y
Gauss	10°	REC	XX	Y
Trapezoid	10°	REC	XX	Y
Boxcar	10°	REC	3°	Y

- 1032 Table 2: SP_dKS waveform library parameter space used in the pilot case study. The
- 1033 V_p, V_s, and density values are set to -10%, -30%, +10% relative to the PREM model
- 1034 of Dziewonski and Anderson (1981) respectively. The left-edge interval is 2.5^o
- 1035 unless otherwise stated.
- 1036

Length (^o)	Shape	ULVZ	Near edge Range
		Height (km)	Co-latitude (º)
1.25	Boxcar, Gaussian, Trapezoid	10	5-30
2.5	Boxcar, Gaussian, Trapezoid	10	5-30, 75-110
3	Boxcar	10	5-21 (1º interval)
5	Boxcar, Gaussian, Trapezoid	10	5-30, 75-110
7.5	Boxcar, Gaussian, Trapezoid	10	5-30, 75-110
10	Boxcar, Gaussian, Trapezoid	10	5-30, 75-110
180 (1D ULVZ)	N/A	10	0
>40 (sided ULVZ)	N/A	10	0, 60
0 (PREM)	N/A	N/A	N/A

1037